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# Quinoxalin-2-yl *o*-tolyl ether

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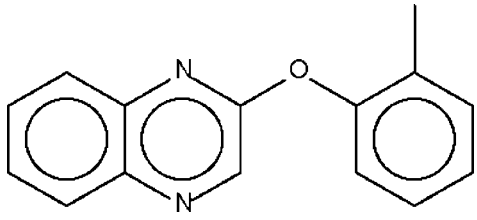
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.004 Å; disorder in main residue; $R$ factor = 0.066; $wR$ factor = 0.184; data-to-parameter ratio = 12.1.

The dihedral angle between the two aromatic ring systems in the title compound, $C_{15}H_{12}N_2O$, is 85.9 (1)°; The angle at the O atom is widened to 118.2 (2)°. The quinoxalinyloxy part of the molecule lies on a mirror plane and the tolyl group is disordered over two positions about the mirror plane.

## Related literature

The title compound exhibits fluorescence; see: Abdullah (2005); Kawai *et al.* (2001); Mohd Salleh *et al.* (2007).




## Experimental

### Crystal data

$C_{15}H_{12}N_2O$
$M_r$ = 236.27
Monoclinic, $P2_1/m$
$a$ = 7.874 (2) Å
$b$ = 7.413 (1) Å
$c$ = 10.596 (2) Å
$\beta$ = 108.332 (3)°
$V$ = 587.1 (2) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 100 (2) K
0.20 × 0.20 × 0.08 mm

### Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
3392 measured reflections
1443 independent reflections
1032 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.183
$S$ = 1.03
1443 reflections
119 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2769).

## References

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# supporting information

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## Quinoxalin-2-yl *o*-tolyl ether

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### S1. Experimental

*o*-Cresol (0.54 g, 5 mmol) was dissolved in a small volume of water containing potassium hydroxide (0.20 g, 5 mmol). The mixture was heated to remove the water to give a brown compound. The compound and 2-chloroquinoxaline (0.82, g, 5 mmol) were heated in THF (15 ml) for 8 h. The mixture was in 1 N sodium hydroxide; the aqueous solution was extracted with dichloromethane. The organic phase was dried over sodium sulfate. Evaporation of the solvent gave a yellow product, which was was washed with chloroform to remove impurities. Crystals were obtained upon recrystallization from an ethyl acetate/hexane mixture.

### S2. Refinement

The tolyl group is disordered about a mirror plane; the phenylene ring was refined as a rigid hexagon. The seven carbon atoms were allowed to refine off the symmetry element; the atoms were all given 0.5 site occupancy.

H-atoms were placed in calculated positions (C—H 0.95–0.98 Å) and were included in the refinement in the riding model approximation, with $U$(H) fixed at 1.2–1.5$U$(C).

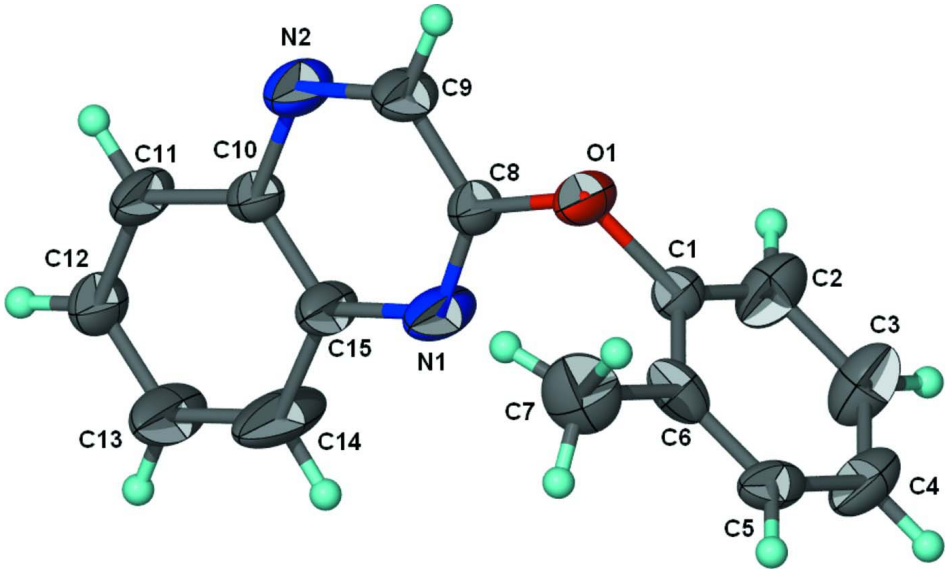


**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of $C_{15}H_{12}N_2O$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

## Quinoxalin-2-yl *o*-tolyl ether

*Crystal data*

$C_{15}H_{12}N_2O$
$M_r = 236.27$
Monoclinic, $P2_1/m$
Hall symbol: -P 2yb
$a = 7.874$ (2) Å
$b = 7.413$ (1) Å
$c = 10.596$ (2) Å
$\beta = 108.332$ (3)°
$V = 587.1$ (2) Å$^3$
$Z = 2$
$F(000) = 248$
$D_x = 1.337$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 756 reflections
$\theta = 2.7$–$24.6°$
$\mu = 0.09$ mm$^{-1}$
$T = 100$ K
Block, colorless
0.20 × 0.20 × 0.08 mm

*Data collection*

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
3392 measured reflections
1443 independent reflections
1032 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.0°$
$h = -10 \rightarrow 8$
$k = -9 \rightarrow 8$
$l = -12 \rightarrow 13$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.183$
$S = 1.03$
1443 reflections
119 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0776P)^2 + 0.4106P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å$^{-3}$
$\Delta\rho_{min} = -0.31$ e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| O1 | 0.1778 (2) | 0.2500 | 0.64890 (18) | 0.0405 (6) | |
| N1 | 0.4752 (3) | 0.2500 | 0.7791 (2) | 0.0552 (9) | |
| N2 | 0.3518 (3) | 0.2500 | 0.9997 (2) | 0.0479 (8) | |
| C1 | 0.2266 (3) | 0.1943 (3) | 0.5368 (2) | 0.0256 (8) | 0.50 |
| C2 | 0.2256 (5) | 0.0171 (3) | 0.4936 (3) | 0.047 (2) | 0.50 |
| H2 | 0.2002 | −0.0787 | 0.5445 | 0.056* | 0.50 |
| C3 | 0.2619 (5) | −0.0199 (3) | 0.3761 (3) | 0.0473 (11) | 0.50 |
| H3 | 0.2612 | −0.1410 | 0.3466 | 0.057* | 0.50 |
| C4 | 0.2991 (4) | 0.1203 (4) | 0.3017 (2) | 0.0417 (12) | 0.50 |
| H4 | 0.3239 | 0.0950 | 0.2213 | 0.050* | 0.50 |
| C5 | 0.3000 (3) | 0.2975 (3) | 0.3449 (2) | 0.0345 (15) | 0.50 |
| H5 | 0.3255 | 0.3933 | 0.2940 | 0.041* | 0.50 |
| C6 | 0.2638 (3) | 0.3345 (3) | 0.4624 (3) | 0.0313 (8) | 0.50 |
| C7 | 0.2599 (11) | 0.5228 (12) | 0.5056 (7) | 0.0496 (17) | 0.50 |

| | | | | | |
|---|---|---|---|---|---|
| H7A | 0.3449 | 0.5946 | 0.4761 | 0.074* | 0.50 |
| H7B | 0.2932 | 0.5272 | 0.6028 | 0.074* | 0.50 |
| H7C | 0.1391 | 0.5719 | 0.4666 | 0.074* | 0.50 |
| C8 | 0.3083 (3) | 0.2500 | 0.7686 (2) | 0.0300 (6) | |
| C9 | 0.2449 (4) | 0.2500 | 0.8784 (3) | 0.0393 (8) | |
| H9 | 0.1194 | 0.2500 | 0.8633 | 0.047* | |
| C10 | 0.5314 (3) | 0.2500 | 1.0167 (2) | 0.0284 (6) | |
| C11 | 0.6553 (4) | 0.2500 | 1.1448 (3) | 0.0429 (8) | |
| H11 | 0.6135 | 0.2500 | 1.2197 | 0.051* | |
| C12 | 0.8343 (4) | 0.2500 | 1.1638 (3) | 0.0398 (8) | |
| H12 | 0.9169 | 0.2500 | 1.2513 | 0.048* | |
| C13 | 0.8952 (4) | 0.2500 | 1.0547 (3) | 0.0631 (12) | |
| H13 | 1.0201 | 0.2500 | 1.0674 | 0.076* | |
| C14 | 0.7769 (4) | 0.2500 | 0.9289 (3) | 0.0889 (19) | |
| H14 | 0.8209 | 0.2500 | 0.8551 | 0.107* | |
| C15 | 0.5922 (3) | 0.2500 | 0.9066 (3) | 0.0378 (7) | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0199 (9) | 0.0771 (16) | 0.0236 (9) | 0.000 | 0.0055 (7) | 0.000 |
| N1 | 0.0196 (11) | 0.123 (3) | 0.0224 (12) | 0.000 | 0.0065 (9) | 0.000 |
| N2 | 0.0248 (12) | 0.093 (2) | 0.0270 (12) | 0.000 | 0.0090 (9) | 0.000 |
| C1 | 0.0198 (14) | 0.033 (2) | 0.0229 (16) | 0.0038 (12) | 0.0051 (12) | 0.0008 (12) |
| C2 | 0.057 (4) | 0.056 (5) | 0.031 (3) | 0.004 (3) | 0.018 (3) | 0.002 (3) |
| C3 | 0.072 (3) | 0.041 (3) | 0.032 (2) | 0.015 (2) | 0.021 (2) | 0.0047 (19) |
| C4 | 0.040 (2) | 0.064 (4) | 0.024 (2) | 0.015 (2) | 0.0142 (17) | 0.002 (2) |
| C5 | 0.0231 (15) | 0.054 (5) | 0.0263 (17) | −0.0015 (15) | 0.0075 (13) | 0.0121 (16) |
| C6 | 0.0175 (15) | 0.0301 (19) | 0.039 (2) | −0.0008 (15) | −0.0015 (15) | 0.0020 (17) |
| C7 | 0.055 (3) | 0.037 (3) | 0.054 (4) | −0.001 (3) | 0.013 (3) | 0.008 (3) |
| C8 | 0.0220 (12) | 0.0435 (16) | 0.0233 (12) | 0.000 | 0.0053 (10) | 0.000 |
| C9 | 0.0188 (12) | 0.069 (2) | 0.0304 (14) | 0.000 | 0.0084 (11) | 0.000 |
| C10 | 0.0230 (12) | 0.0369 (15) | 0.0259 (13) | 0.000 | 0.0086 (10) | 0.000 |
| C11 | 0.0303 (14) | 0.076 (2) | 0.0227 (13) | 0.000 | 0.0093 (11) | 0.000 |
| C12 | 0.0265 (14) | 0.065 (2) | 0.0243 (13) | 0.000 | 0.0020 (11) | 0.000 |
| C13 | 0.0211 (14) | 0.137 (4) | 0.0291 (15) | 0.000 | 0.0053 (12) | 0.000 |
| C14 | 0.0238 (15) | 0.221 (6) | 0.0247 (16) | 0.000 | 0.0111 (13) | 0.000 |
| C15 | 0.0218 (13) | 0.067 (2) | 0.0236 (13) | 0.000 | 0.0063 (10) | 0.000 |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C8 | 1.359 (3) | C6—C7 | 1.472 (9) |
| O1—C1 | 1.420 (3) | C7—H7A | 0.9800 |
| O1—C1$^{i}$ | 1.420 (3) | C7—H7B | 0.9800 |
| N1—C8 | 1.283 (3) | C7—H7C | 0.9800 |
| N1—C15 | 1.375 (3) | C8—C9 | 1.402 (4) |
| N2—C9 | 1.296 (4) | C9—H9 | 0.9500 |
| N2—C10 | 1.369 (3) | C10—C15 | 1.392 (4) |

| | | | |
|---|---|---|---|
| C1—C2 | 1.3900 | C10—C11 | 1.400 (4) |
| C1—C6 | 1.3900 | C11—C12 | 1.360 (4) |
| C2—C3 | 1.3900 | C11—H11 | 0.9500 |
| C2—H2 | 0.9500 | C12—C13 | 1.384 (4) |
| C3—C4 | 1.3900 | C12—H12 | 0.9500 |
| C3—H3 | 0.9500 | C13—C14 | 1.365 (4) |
| C4—C5 | 1.3900 | C13—H13 | 0.9500 |
| C4—H4 | 0.9500 | C14—C15 | 1.398 (4) |
| C5—C6 | 1.3900 | C14—H14 | 0.9500 |
| C5—H5 | 0.9500 | | |

| | | | |
|---|---|---|---|
| C8—O1—C1 | 117.19 (19) | O1—C8—C9 | 114.4 (2) |
| C8—N1—C15 | 115.8 (2) | N2—C9—C8 | 122.2 (2) |
| C9—N2—C10 | 116.9 (2) | N2—C9—H9 | 118.9 |
| C2—C1—C6 | 120.0 | C8—C9—H9 | 118.9 |
| C2—C1—O1 | 125.13 (17) | N2—C10—C15 | 120.2 (2) |
| C6—C1—O1 | 114.68 (17) | N2—C10—C11 | 120.2 (2) |
| C1—C2—C3 | 120.0 | C15—C10—C11 | 119.6 (2) |
| C1—C2—H2 | 120.0 | C12—C11—C10 | 121.2 (3) |
| C3—C2—H2 | 120.0 | C12—C11—H11 | 119.4 |
| C2—C3—C4 | 120.0 | C10—C11—H11 | 119.4 |
| C2—C3—H3 | 120.0 | C11—C12—C13 | 119.4 (3) |
| C4—C3—H3 | 120.0 | C11—C12—H12 | 120.3 |
| C5—C4—C3 | 120.0 | C13—C12—H12 | 120.3 |
| C5—C4—H4 | 120.0 | C14—C13—C12 | 120.4 (3) |
| C3—C4—H4 | 120.0 | C14—C13—H13 | 119.8 |
| C4—C5—C6 | 120.0 | C12—C13—H13 | 119.8 |
| C4—C5—H5 | 120.0 | C13—C14—C15 | 121.3 (3) |
| C6—C5—H5 | 120.0 | C13—C14—H14 | 119.4 |
| C5—C6—C1 | 120.0 | C15—C14—H14 | 119.4 |
| C5—C6—C7 | 119.7 (3) | N1—C15—C10 | 121.5 (2) |
| C1—C6—C7 | 120.3 (3) | N1—C15—C14 | 120.4 (2) |
| N1—C8—O1 | 122.3 (2) | C10—C15—C14 | 118.1 (3) |
| N1—C8—C9 | 123.4 (2) | | |

| | | | |
|---|---|---|---|
| C8—O1—C1—C2 | 87.53 (18) | $C1^{i}$—O1—C8—C9 | 160.91 (12) |
| $C1^{i}$—O1—C1—C2 | −173.48 (14) | C10—N2—C9—C8 | 0.000 (2) |
| C8—O1—C1—C6 | −97.56 (16) | N1—C8—C9—N2 | 0.000 (2) |
| $C1^{i}$—O1—C1—C6 | 1.43 (19) | O1—C8—C9—N2 | 180.000 (1) |
| C6—C1—C2—C3 | 0.0 | C9—N2—C10—C15 | 0.000 (2) |
| O1—C1—C2—C3 | 174.7 (2) | C9—N2—C10—C11 | 180.000 (2) |
| C1—C2—C3—C4 | 0.0 | N2—C10—C11—C12 | 180.000 (2) |
| C2—C3—C4—C5 | 0.0 | C15—C10—C11—C12 | 0.000 (2) |
| C3—C4—C5—C6 | 0.0 | C10—C11—C12—C13 | 0.000 (2) |
| C4—C5—C6—C1 | 0.0 | C11—C12—C13—C14 | 0.000 (2) |
| C4—C5—C6—C7 | −178.3 (4) | C12—C13—C14—C15 | 0.000 (2) |
| C2—C1—C6—C5 | 0.0 | C8—N1—C15—C10 | 0.000 (1) |
| O1—C1—C6—C5 | −175.2 (2) | C8—N1—C15—C14 | 180.000 (1) |

| | | | |
|---|---|---|---|
| C2—C1—C6—C7 | 178.2 (4) | N2—C10—C15—N1 | 0.000 (2) |
| O1—C1—C6—C7 | 3.0 (4) | C11—C10—C15—N1 | 180.000 (1) |
| C15—N1—C8—O1 | 180.000 (1) | N2—C10—C15—C14 | 180.000 (2) |
| C15—N1—C8—C9 | 0.000 (1) | C11—C10—C15—C14 | 0.000 (2) |
| C1—O1—C8—N1 | 19.09 (12) | C13—C14—C15—N1 | 180.000 (2) |
| C1$^{i}$—O1—C8—N1 | −19.09 (12) | C13—C14—C15—C10 | 0.000 (2) |
| C1—O1—C8—C9 | −160.91 (12) | | |

Symmetry code: (i) $x$, $-y+1/2$, $z$.